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Studying the Infrared Spectroscopy of the SnO_2:Sb (x = 0.00, 0.03) Powders

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Abstract
The nanocrystals of semiconducting metal oxides have attracted great attention because of their interesting properties. Therefore, our study of some physical properties of the pure and Sb doping Tin Oxide powder , The measurement of the infrared spectrum of pure tin oxide powder shows vibrational frequencies (415.585 - 574.683 - 1641.13 – 2125.3- 3432.67) cm^{-1} and for Sb doping tin oxide ;(x=0.03) shows vibration frequencies and the most prominent is (573.719 – 941.092 – 1384.64 – 1637.27 – 3415.56) cm^{-1} , the study showed that the greatest value of the absorbance and absorption coefficient was in doping sample respectively A = 0.819, α = 18.839 cm^{-1} corresponding to the wavenumber υ = 573.719 cm^{-1}, the greatest value of the optical conductivity was in pure sample $0.0831(\Omega cm)^{-1}$ corresponding to the wavenumber υ = 3432.67 cm^{-1} and the refractive index for pure tin oxide ranged from [1.832 - 2.371]. As for the Sb doping Tin Oxide powder, the refractive index value was between [1.122 – 2.152].
Keywords: Tin Oxide - infrared spectrum - absorbance - absorption coefficient - refractive index - optical conductivity.
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1. Introduction

Tin oxide (SnO2) is one of the most important n-type metal oxide semiconductors with wide band gap (3.6 eV at 300 K) [1]. Because of its unique electronic, optical, electrochemical and catalytic properties, it has been widely used in flat panel displays, transparent conducting electrodes,solar cells, gas sensors and rechargeable Li-ion batteries, etc. [2]. The interest in SnO2 is evinced because it is a naturally non-stoichiometry prototype transparent conducting oxide (TCO) having high transparency in visible region and high reflectivity in IR region. Further, the electrical resistance of SnO2 is small [3]. High infrared _IR_ reflectivity is one of the key requirements for high-quality window materials and architectural glass, which can prevent heat exchange in the form of IR radiation . The IR reflectivity of stoichiometric SnO2 is low because of its low intrinsic free carrier concentration and mobility, which are thought to be due to doubly ionized vacancies serving as donors [4].

Dopings with fluorine (F), indium (In) and antimony (Sb) are used to improve its optical properties and conductivity [5-7].

SnO_2 has tetragonal structure belonging to the P42/mnm space group. The lattice parameters are a = b = 4.7382 and c = 3.1871 A [8]. Its unit cell contains two tin and four oxygen atoms as is shown in figure (1) . The tin atom is at the center of six oxygen atoms placed at the corners of a regular octahedron. Every oxygen atom is surrounded by three tin atoms at the corners of an equilateral triangle [9].

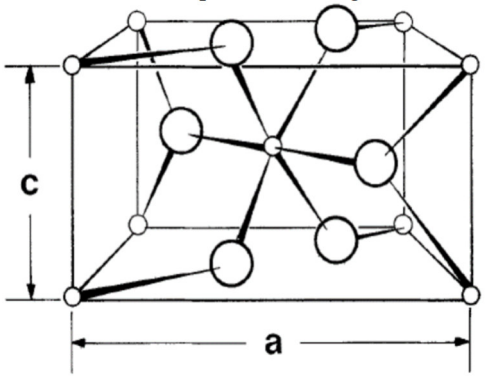

Fig (1): Unit cell of the crystal structure of SnO_2. Large circles indicate oxygen atoms and the small circles indicate tin atoms .

2. Infrared spectroscopy

Infrared is electromagnetic waves and it has all the basic properties of light, which are represented by the phenomena of diffusion, reflection, refraction, interference, diffraction and polarization. They are invisible thermal

waves emitted by the sun or from artificial sources and have a high penetration ability as well as from our bodies and their frequency is lower than the red ray frequency in the visible electromagnetic spectrum. The infrared spectrum is located between the visible spectrum and the microwave radiation spectrum. It is divided into three zones, as follows:

- Near infrared (NIR): It is the closest to the visible rays, namely the red color, and it lies within the range [4000 - 12000] cm^{-1} .
- Middle Infrared MIR: located between the two preceding zones within the range [200 -4000] cm^{-1} .
- Infrared spectroscopy is one of the basic methods of studying materials. It enables us to identify the structure of the material without affecting its properties. It depends on the study of the spectra absorbed by the sample, and its field is limited to [20 -1400] cm^{-1} .

Red radiation energy is not enough to cause electronic excitation in most materials, but it is sufficient to cause elasticity vibrations and flexion in the bonds. All types of these bonds respond to this amount of energy in which vibrations of this type occur. Therefore, they are absorbed in the zone beneath the red under the condition that absorption leads to a change in the polar moment, and these vibrations are quantized, and their occurrence means that the compound absorbs infrared energy in a specific part of the spectrum. [10]

Most spectroscopic analysis occur in the central infrared zone [20 – 1400] cm^{-1} where the most molecular vibrations occur to determine the molecular structure of the studied compounds.

3. Infrared spectroscopy principle

Natural molecules vibrate according to all their vibrating patterns, but with very weak amplitudes. However, the photon has a sinusoidal electric component. If the frequency of the photon corresponds to the frequency of the vibrations of the normal patterns of the molecule, the molecule will enter the resonance and vibrate at very large capacities. In other words the photon whose energy is Equal to the energy necessary for the molecule to pass from a low energy state to an excited state is absorbed and its energy is transformed into a vibration energy as in Figure (2).

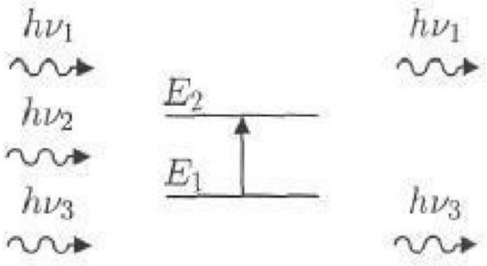

Figure (2) : Infrared absorption .

Only the photon whose energy (hv) equals to the transmission energy (E2-E1) is absorbed and thus the emission of the emitted radiation is impaired. As the absorption of some of the incoming photons leads to the appearance of the lines of compatibility of the photons that were not emitted in the curve of the infrared spectrum of the molecule. This absorption distinguishes the bonds between the atoms, since each vibration pattern corresponds to the single movement of the molecule, so there is a direct correspondence between the frequency of the absorbed radiation and the structure of the molecule [11].

Research objective:

This work aims to determine the field of absorption frequencies, that is the vibrations samples frequencies of the infrared spectra of pure tin oxide and antimony doped tin oxide by (3wt%), and then finding the absorbance, reflectance , absorption coefficient, damping factor, refractive index, optical length and optical conductivity to improve the physical properties of tin oxide.

Research materials and methods:

The following materials have been used in preparing the samples:

- Tin oxide SnO_2 (99% purity, TITAN BIOTECH LTD, origin India).
- Antimony Sb (99% purity, TITAN BIOTECH LTD, origin India).

Devices and tools used:

1- Sensitive scale type (SARTORIUS) with an accuracy of (10^{-4}) gr is available in the Faculty of Science - Physics Department.
2- Small agate mortar.
3- High temperature thermal Oven (1200°C) with a Temperature Regulator.

4- Preparing the samples:

The samples are prepared by the solid state reaction method. Accordingly the weights of the powders required for each sample are mixed and calculated using the molecular weight method in order to obtain the compounds required for the study where $Sn_{1-x}Sb_xO_2$; (x= 0.00 - 0.03). Then grinding these materials in the agate mortar perfectly well to make the mixture homogeneous and sifting it with a sieve of 90 µm. Then it is put it in a container and we add distilled water to increase the mixing process and homogeneity of the powder. Then we put it on a heater for 3 hours at a temperature of 100° C and the mixing and homogeneity process of the powder occurs by stirring.

After that, the powder is placed on a heater with direct contact with the air, then the water evaporates and then we perform a preliminary roasting process inside the oven (pre-sinter) to increase the degree of homogeneity of the mixture. We fix the oven temperature at 700°C for three hours, then we turn off the oven, which means to stop the roasting process and leave the sample inside the oven until it cools and reaches room temperature, thus we get rid of impurities that evaporate at high temperatures.

Then we grind the powder resulting from the roasting process in its first stage. Then we perform the second roasting process where we fix the oven temperature at 100° C for an hour and then we raise the temperature 50°C every 15min until we reach the temperature of 700°C where we fix the oven temperature at it for 3 hours In order to get the crystal structure in its correct form.

To study the infrared spectra, we use an infrared spectroscopy device, which is a simple device whose main components are an infrared source, a sample holder and a detector. This device is considered one of the best spectroscopic devices used to identify the chemical composition of the compounds. It is available in the Faculty of Science - Tishreen University works at the range [400-4000] cm^{-1}.

The spectrometer is characterized by a computer memory that analyzes the waves gathered on the detector, computerizes them, and draws the spectrum resulting from absorption. Or a vibratory transmission of the atoms occurs relative to each other in the molecule, which leads to a periodic change in the length of chemical bonds or a change in the angles between the chemical bonds in the molecule. Each vibrational motion results from the movement of two atoms, or it may include a group of its constituent atoms. The wavelength or frequency at which this absorption occurs depends on several factors, including the mass of the atom, the strength of the bonds that make up the molecule, and the geometry of the atoms in the molecule.

5- Results and discussion:

The IR spectrum of pure tin oxide and antimony doped tin oxide was measured using the spectrometer **asco** type **FT / IR-460 plus** available in the central laboratory of the Faculty of Science - Tishreen University, working in the range [400-4000] cm^{-1}. Where the permeability T was measured by the frequency function υ , the absorbance A, the reflectance R, the absorption coefficient α, the damping factor K, the refractive index n and optical conductivity σ_{opt} were calculated:

1- **Permeability T**: It is defined as the ratio between the intensity of the penetrating radiation to the intensity of the fallen radiation, it has been taken from the device itself and then by using the appropriate mathematical equations, other optical parameters have been calculated.

2- **Absorbency A**: is the ratio between the intensity of the absorbed radiation and the intensity of the fallen radiation, calculated from the equation [12]:

$$A = \log\left(\frac{100}{T\%}\right) = \log\left(\frac{1}{T}\right) \qquad (1)$$

Trepresents Permeability.

3- **Reflectance R** : is the ratio between the intensity of the reflected radiation and the intensity of the fallen radiation , calculated from the equation [13] :

$$R+T+A=1 \qquad (2)$$

4- **Absorption coefficient α**: defined as the ratio between the decrease in the flow of the fallen radiation energy to the unit of distance towards the spread of the fallen light wave within the field, and is calculated from the equation [14] :

$$\alpha = 2.303\frac{A}{d} \qquad (3)$$

A represents absorbency , d = 1mm the thickness of the material

5- **The damping factor k**: is defined as the amount of energy absorbed by the electrons of the studied material from the energy of the radiation photons that fall on it, and is calculated from the equation [15]:

$$k = \frac{\alpha}{4\pi\nu} \qquad (4)$$

6- **Refractive index n**: which is the ratio between the speed of light in the vacuum to its speed in the field, and it is calculated from the equation [16] :

$$n = \left[\left(\frac{1+R}{1-R}\right)^2 - (K^2+1)\right]^{1/2} + \frac{1+R}{1-R} \qquad (5)$$

R represents reflectance .

7- **Optical length L**: the inversion of the absorption coefficient [14]:

$$L = \frac{1}{\alpha} \qquad (6)$$

8- **Optical conductivity σ_{opt}**: optical conductivity is related to the refractive index and the damping factor according to the following equation [17]:

$$\sigma_{opt} = \frac{1}{30} nk\nu \qquad (7)$$

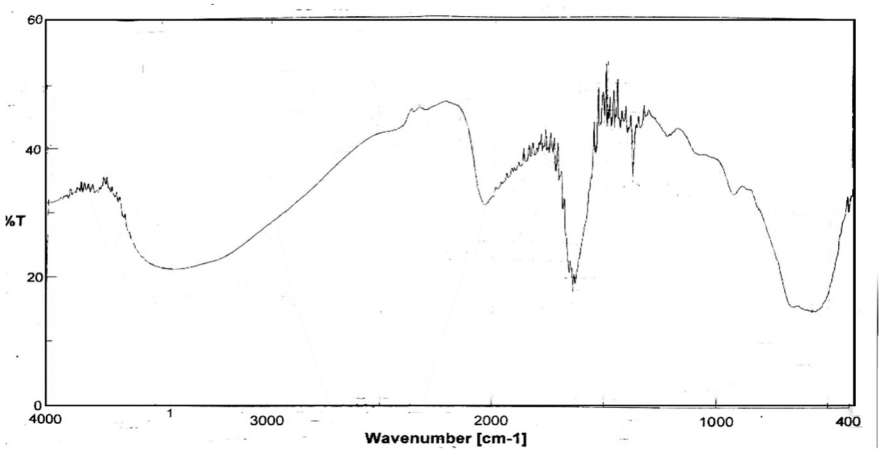

Figure (3): Represents the FTIR spectrum for pure tin oxide.

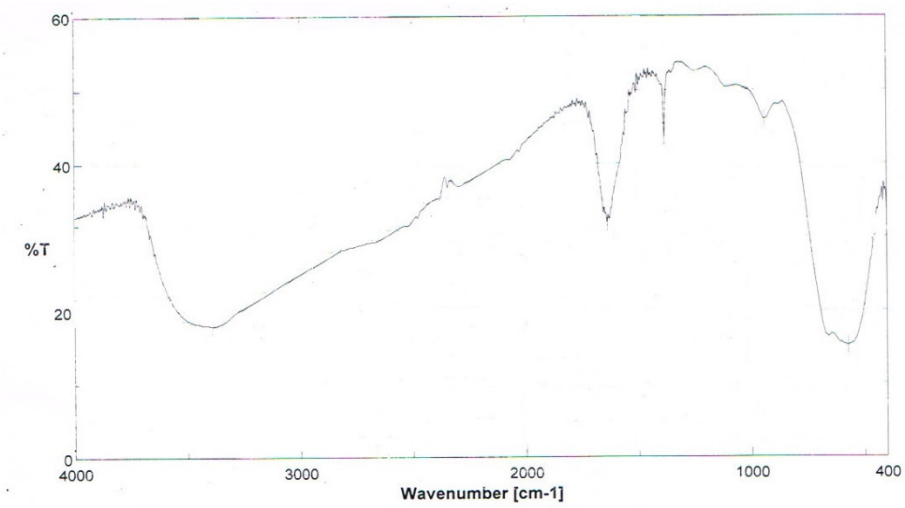

Figure (4): Represents FTIR spectrum of antimony doped tin oxide by (3wt%).

FTIR is a technique used to obtain information regarding chemical bonding and functional groups in a material. In the transmission mode, it is quite useful to predict the presence of certain functional groups which are adsorbed at certain frequencies; thus, it reveals the structure of the material. The band positions and numbers of absorption peaks depend on the crystalline structure, chemical composition, and also on morphology [18]. To investigate chemical groups on the surface of sintered samples, an FTIR analysis was carried out at room temperature over the wave number range of 400– 4000 cm^{-1}. The broad absorption band at 3432.67 cm^{-1}, and 1641.13 cm^{-1} are assigned to the vibration of hydroxyl group due to the absorbed/adsorbed water and show a stretching vibrational mode of O–H group [19]. the main IR features of SnO2 appear at 415.58 and 574.62 cm^{-1} . which assign to O – Sn – O and Sn – O stretching vibration , respectively [20]. The changing in the shapes and positions of absorption peaks indicates to presence of stretching modes, which are, give an indication of successful doping Sb to tin oxide nanoparticles [21].

Pure tin oxide is characterized by a set of vibrational frequencies within the range [400-4000] cm^{-1} which is: (3432.67 – 2125.3 – 1641.13 – 574.683 – 415.585) cm^{-1} .

Antimony doped tin oxide by (3wt%) is characterized by a set of vibrational frequencies within the range [400-4000] cm^{-1} which is: (3415.56 – 1637.27 – 1384.64 – 941.92 – 573.719) cm^{-1}.

Table: (1) shows the vibrations frequency of pure tin oxide with corresponding permeability values for each frequency, absorbance, reflectance , absorption coefficient, damping factor, refractive index, optical length and

optical conductivity.

ν (cm)$^{-1}$	T%	A	R	α (cm)$^{-1}$	k	n	L(cm)	$\sigma_{(opt)}$(Ω.cm)$^{-1}$
3432.67	21.092	0.6758	0.1131	15.54529	0.000361	2.014	0.0643	0.083093
2125.3	27.692	0.5576	0.1654	12.82585	0.00048	2.371	0.0779	0.080712
1641.13	18.841	0.7248	0.0866	16.67261	0.000809	1.834	0.05997	0.081178
574.683	18.813	0.7255	0.0863	16.68746	0.002312	1.832	0.05992	0.08114
415.585	20.188	0.6949	0.1032	15.98285	0.003062	1.946	0.0625	0.082572

Table: (2) shows the vibrations frequency of the antimony doped tin oxide by (3 wt%) with corresponding permeability values for each frequency, absorbance , reflectance, absorption coefficient, damping factor, refractive index, optical length and optical conductivity.

ν (cm)$^{-1}$	T%	A	R	α (cm)$^{-1}$	k	n	L(cm)	$\sigma_{(opt)}$(Ω.cm)$^{-1}$
3415.56	18.502	0.7327	0.0822	16.8539	0.000393	1.374	0.0593	0.061470
1637.27	31.878	0.4964	0.1847	11.4194	0.000555	2.008	0.0875	0.060883
1384.64	43.539	0.3611	0.2034	8.3057	0.000478	2.152	0.1203	0.047445
941.92	46.052	0.3367	0.2027	7.7452	0.000655	2.146	0.1291	0.044120
573.719	15.166	0.8191	0.0292	18.8397	0.002614	1.122	0.0530	0.056108

Figure (5) shows the change in the absorbance of pure and antimony doped tin oxide , we note that the largest absorbance value corresponds to the Sb doped tin oxide at the value 0.819 corresponding to the wavenumber (573.719) cm $^{-1}$, and the smallest value of absorbance corresponds to the Sb doped tin oxide at the value 0.336 corresponding to the wavenumber (941.092) cm^{-1}.

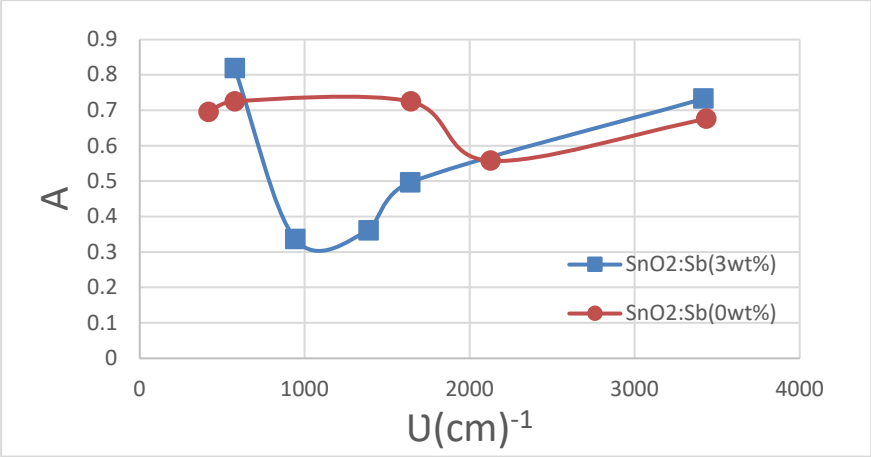

Figure (5): the absorbance by the wavenumber function of pure SnO_2 and Sb doped SnO_2 powder by (3wt%) .

The absorption coefficient variations have been studied by the frequency function as in Figure (6), and that the largest value absorption coefficient corresponds to the Sb doped tin oxide at the value 18.839 cm^{-1} corresponding to the wavenumber 573.719cm $^{-1}$, and the smallest value of absorption coefficient corresponds to the Sb doped tin oxide at the value 7.745 cm^{-1} corresponding to the wavenumber 941.092 cm^{-1}.

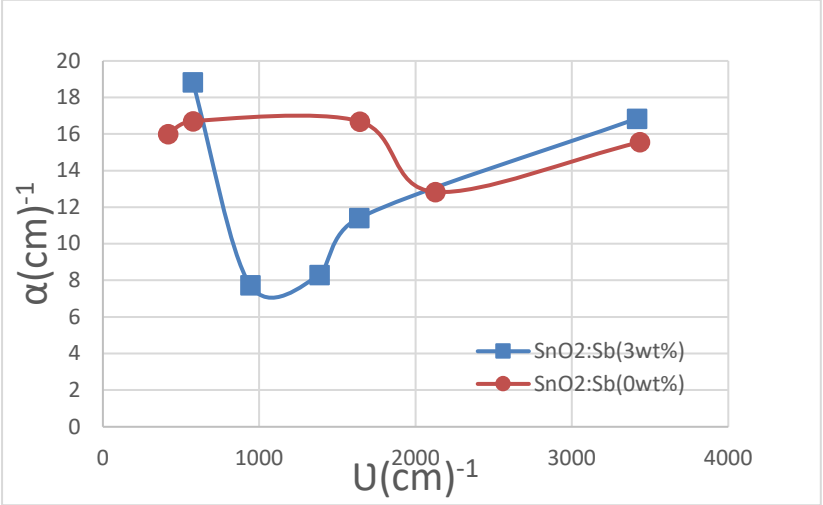

Figure (6): the absorption coefficient by the wavenumber function of pure SnO_2 and Sb doped SnO_2 powder by (3wt%) .

Figure (7) shows the refractive index of the pure tin oxide and Sb doped tin oxide by (3wt%) powder , where the values of the refractive index in the pure sample ranges between [1.832-2.371] . we notice the smallest value of refractive index corresponds to the Sb doped tin oxide at the value 1.122 corresponding to the wavenumber 573.719 cm^{-1}.

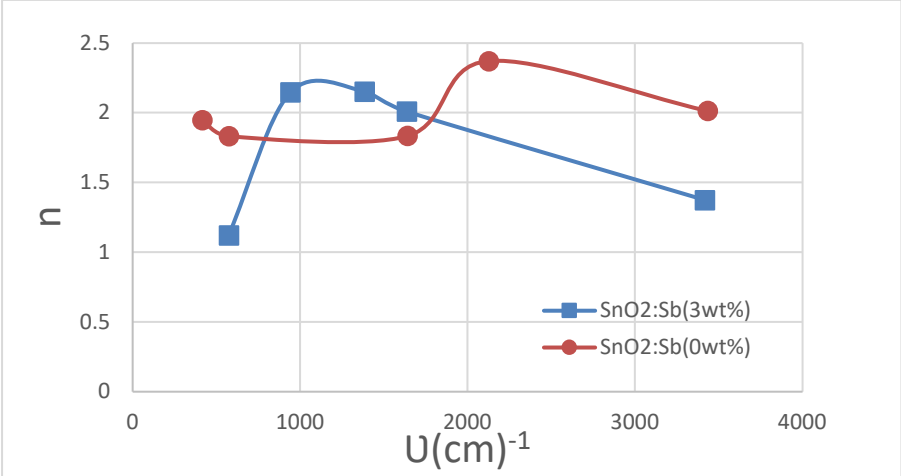

Figure (7): the refractive index by the wavenumber function of pure SnO_2 and Sb doped SnO_2 powder by (3wt%) .

Figure (8) shows the optical conductivity of the pure tin oxide and Sb doped tin oxide by (3wt%) powder , where the values of the optical conductivity in the pure sample ranges between [0.0807-0.0830] $(\Omega cm)^{-1}$.
We also notice an dencrease in the value of the optical conductivity with Sb doping , where the smallest value was at 0.0441 $(\Omega cm)^{-1}$ corresponding to the wave number (941.092) cm^{-1}.

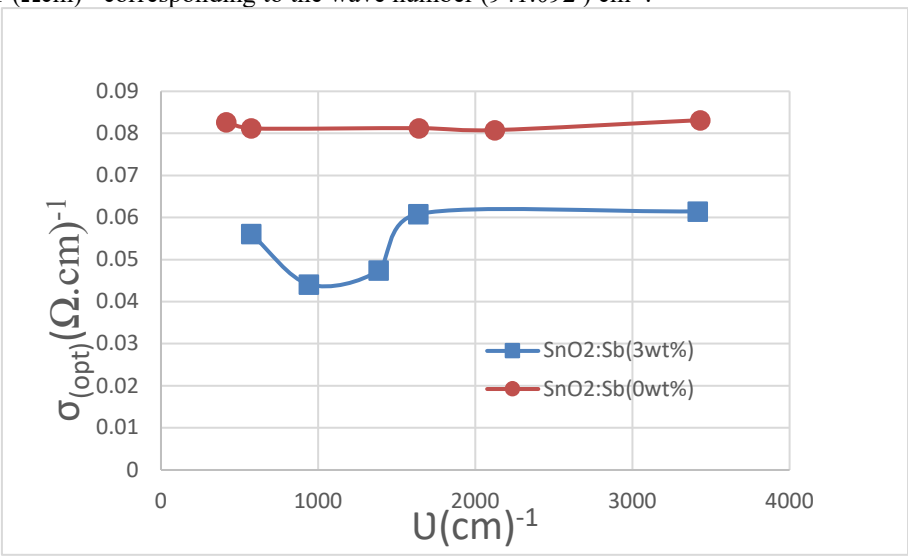

Figure (8): the optical conductivity by the wavenumber function of pure SnO_2 and Sb doped SnO_2 powder by (3wt%) .

Conclusions

1. The pure tin oxide FTIR spectrum has shown some vibrational frequencies within the range [400-4000] cm^{-1} which are (415.585 - 574.683 - 1641.13 – 2125.3- 3432.67) cm^{-1}
2. The FTIR spectrum of the antimony doped tin oxide by 3wt% showed vibrational frequencies within the range [400-4000] cm^{-1}, the most notably are: (573.719 – 941.092 – 1384.64 – 1637.27 – 3415.56) cm^{-1}
3. The absorbance value for the pure sample varies within the range [0.557 – 0.725], and for the doped sample, the absorbance value varies within the range [0.336 – 0.819].
4. The reflectance value varies within the range of the pure sample [0.0863 – 0.1654] , and for the doped sample the reflectance value varies within the range [0.029 – 0.203].
5. The absorption coefficient value varies within the range of the pure sample [12.825 – 16.687] cm^{-1} , and for the doped sample, the absorption coefficient value varies within the range [7.745 – 18.839]cm^{-1}.
6. The value of the refractive index for the pure sample varies within the range [1.832 – 2.371] , and for the doped

sample, the refractive index value varies within the range [1.122 – 2.152].
7. The value of the optical length L concerning the pure sample varies in the range [0.05992 – 0.0779] cm, and for the doped sample the value of the optical length varies within the range [0.053 – 0.1291] cm .
8. The optical conductivity value σ_{opt} for the pure sample varies within the range [0.0807 – 0.0830]$(\Omega cm)^{-1}$, for the doped sample, the value of the optical conductivity varies in the range [0.0441 – 0.0614] $(\Omega cm)^{-1}$.
9. The Fourier transformed infrared (FTIR) spectrum showed a band O – Sn – O and Sn – O stretching vibration .

REFERANCE:

[1] P.G. Li, X. Guo, X.F. Wang, W.H. Tang, (2009) , J. Alloys Compd. 479 , 74–77.
[2] C. Wang, J. Li, Y. Zhang, Y. Wei, J. Liu, (2010) , J. Alloys Compd. 493 , 64–69.
[3] M. Batzill, U. Diebold, Prog. Surf. Sci. 79 , (2005), 47–154.
[4] P. Mitra, A. P. Chatterjee, and H. S. Maiti , (1998) , J. Mater. Sci.: Mater. Electron. **9**, 441.
[5] Ravichandran K, Philominathan P. Mater Lett , (2008) ;62:2980–3.
[6] Ait Aouaj M, Diaz R, Belayachi A, Rueda F, Abd-lefdil M. Mater Res Bull , (2009) ;44: 1458–61.
[7] Feng XJ, Ma J, Yang F, Ji F, Zong FJ, Luan CN, et al. Mater Lett (2008) ;62:1779–81.
[8] -Vadivel S. & Rajarajan G. (2015) "Effect Of Mg Doping On Structural, Optical And Photocatalytic Activity Of SnO2 Nanostructure Thin Films", *Journal of Materials Science*, 6, 730-738.
[9] - Jarzebski Z. & Marton J. (1976), "Physical Properties of SnO2 Materials", Journal of the Electrochemical Society, 199-205.
[10]- ROUESSAC.F, ROUESSAC,A, (2004), AnalyseCHimiqueMéthodes et Techniques Instrumentals Modernes, Dunod, Paris.
[11]- MAGET.V,(2005), Développement de Méthodes de traitement de signaux spectroscopiques: estimation de linge de base et du spectre de raie, Univ Henri Poicré.
[12] SAKNI.L. ,(2017), '' Studying the structural of Fe doped tin oxide'', Master thesis , Alwadi university .
[13] K. L. Chopra, (1985), " Thin Film Phenomena ", Mc. Graw-Hill, New York ,. [13]
[14] AlJAWAD , S. (2016), '' Studying effect of doping on the structural and optical properties of tin oxide thin films'' , Journal of engineering and technology , Vol.34.
[15] MANSOUR, M, (2012),'' Studying the structural and optical properties of ZnO:Cu thin films by APCVD method'' , Vol.5.
[16] S.S Al-Rawi, S. J. Shakir and Y N. Husan, (1990), "Solid State Physics",Pbpublishing of Mousal University Arabic Version .
[17] ZAID, A, (2012), ''Studying the structural and optical properties of NiO thin films'' , Master thesis , Dyala University ,.
[18] Ashokkumar.M,et al, (2014) ," Zn0.96−xCu0.04FexO(0 ⩽ x ⩽ 0.04) alloys – Optical and structural studies), Superlattices and Microstructures, 69, 53-64.
[19] Faisal.M, et al, (2015), "SnO2 doped ZnO nanostructures for highly efficient photocatalyst", Journal of Molecular catalysis A: chemical, 39, 19-25.
[20] Kuantama E, Han DW, Sung YM, Song JE, Han CH. Thin Solid Films. (2009); 517:4211-4.
[21] S.Blessi, M. Maria Lumina Sonia, S.Vijayalakshmi and S.Pauline. (2014) " Preparation and characterization of SnO2 nanoparticles by hydrothermal method", Int. J. of ChemTech Res , 6(3), 2153-2155.